Description for the general public

The presented research project is focused on exploration of the nature of the nitrogen-oxygen bond in a group of aromatic *N*-oxides and possibilities of formation of stable intermolecular complexes with various chemical groups of a Lewis acid character. The main aim of the project is determination of typical *N*-oxide molecular synthons in crystals including their detailed geometrical and energetic characteristics, analysis of potential cooperative/anticoopoerative effects associated with the formation of intermolecular interactions and possibilities of proton transfer reaction through *N*-oxide hydrogen bonding.

The presented project, in its initial stage, is focused analysis of Cambridge Structural Database and synthesis, crystallization and X-ray analysis of novel crystal structures. For description of the analyzed interaction Hirshfeld surface analysis will be used. Infrared spectroscopic analysis in the solid state, especially compared with X-ray results, let assess characteristic absorption bands of *N*-oxide group and study their changes upon intermolecular interactions, especially in of proton transfer. The use of modern methods of computational chemistry let for detailed analysis, classification and description of *N*-oxide intermolecular interactions. Implementation of quantum-chemical calculations for periodic systems allows calculation of lattice energy and its decomposition. There will be also performed a detailed analysis of structural changes of nitrogen-oxygen bond upon intermolecular interactions and their description in the light of modern theories of atomic bonds.

The proposed researches are focused on synthesis of novel *N*-oxide crystal structures, especially multicomponent cocrystals, and identification of phenomena responsible for the stability of resulting molecular complexes. Understanding of the intermolecular forces which govern crystal structure is very important as the first step in molecular self-organization processes and crystal engineering. In this context, the presented project is aimed to broadening existing knowledge of intermolecular interactions.